



BES/Materials Sciences
Center Synthesis Processing

Center of Excellence for Synthesis and Processing **Granular Flow and Kinetics**

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Principal Labs and Investigators

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Plan

- ◆ Flow of granular materials: introduction, issues
- ◆ Center of excellence: goals, organization, budget
- ◆ Center accomplishments: progress report
- ◆ Ongoing research projects





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Granular Flow

Definition of granular material: ensembles of

- ❖ Macroscopic particles (10^{-5} - 10^{-2} m)
- ❖ Hard particles (~1% deformation)
- ❖ Dissipative collisions (~20% energy loss)

Multiphase flows: ubiquitous in industry and in nature

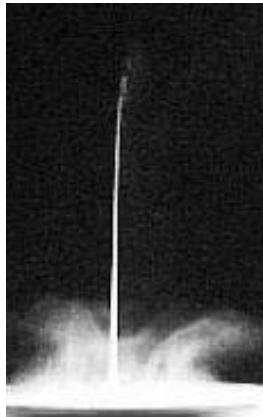
- ❖ Industry: packed/fluidized beds, slurries, powders, grains, explosives, chemical process industry, particle transport
- ❖ Geophysics: sand dune motion, landslides, snow avalanches, flow in porous media, volcanic flows, planetary formation, ...



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Simple system, complex collective phenomena

Dynamics



- ◆ Avalanches
- ◆ Clustering
- ◆ Jamming
- ◆ Fluid interaction

Statics

- ◆ Granular packs
- ◆ Size segregation
- ◆ Cohesion effects
- ◆ Force transmission





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Basic science issues

Stretching the boundaries of mechanics, thermodynamics...

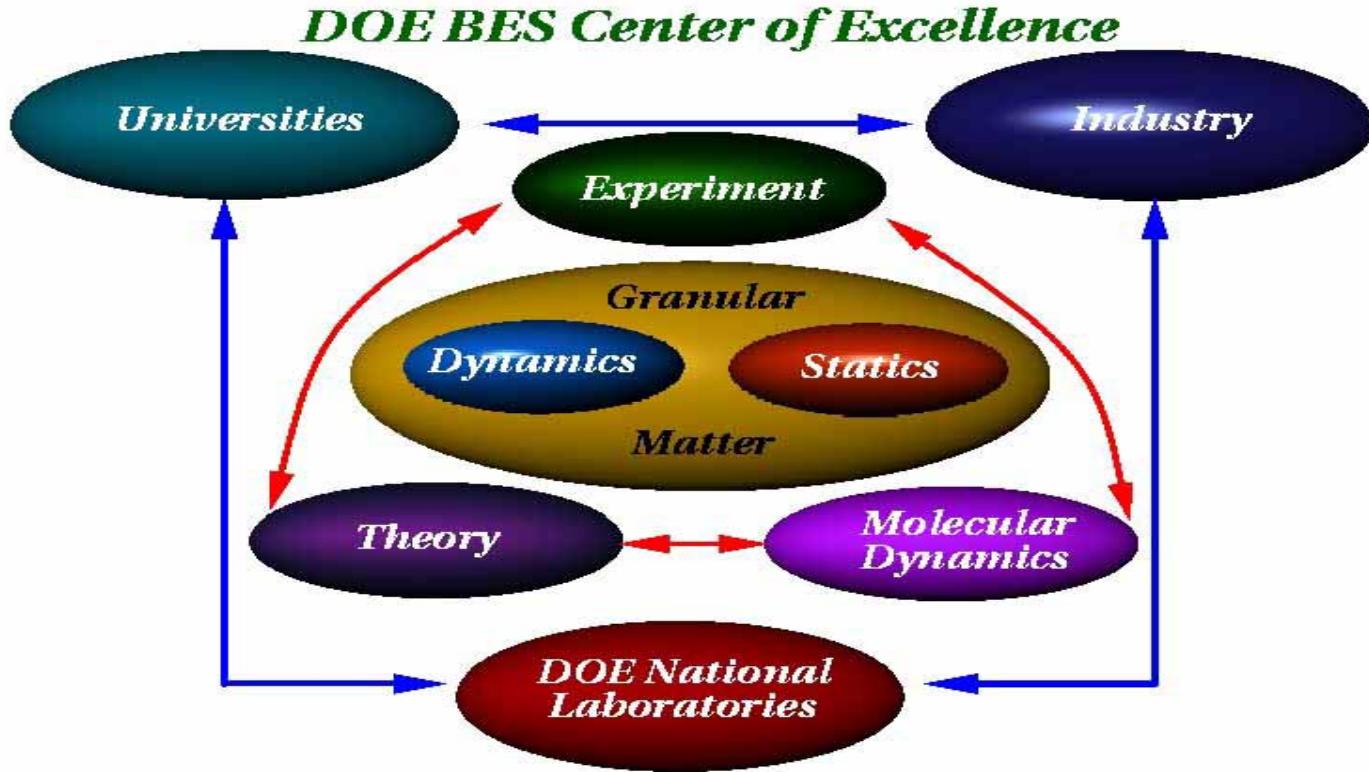
Common Themes	Issues
Extract meso or macroscale behavior from detailed description at particle-level	Flow equations Constitutive relations
Small-scale inhomogeneities in particle field: can they affect macroscale behavior ? Characterize (self-organized?) critical states	Statistical description Pattern characterization Stochastic geometry

- Constitutive relations?
- Equation of state?



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DOE center of excellence





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DOE labs: Leaders in simulation & modeling

Simulation

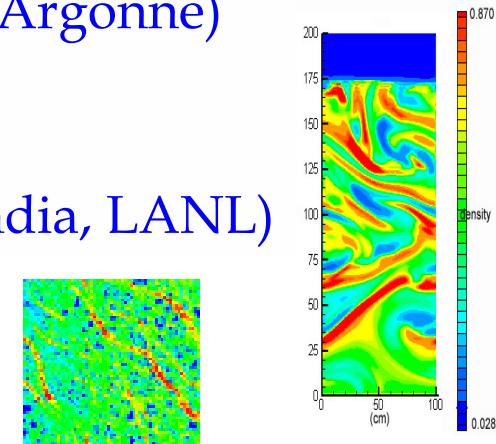
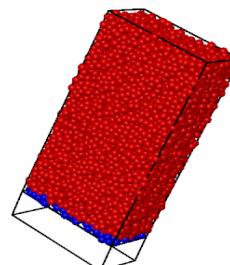
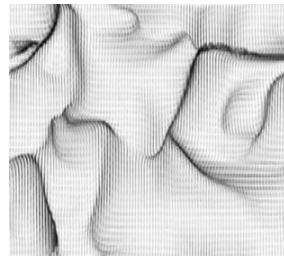
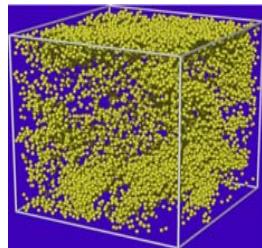
- Molecular Dynamics (soft, hard, parallel) (LANL, SNL, Ames)
- Monte Carlo (LANL, Ames)

Theory

- Continuum mechanics, probabilistic approach (Ames, LANL)
- Kinetic theory, statistical physics (LANL, Ames, Argonne)

Experiment

- Vibration, Shaking, Imaging (LANL, Argonne)
- Electrostatic driving (Argonne), Compaction (Sandia, LANL)





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Center Administration

Executive committee:

Chair: Shankar Subramaniam (Ames)

I Aronson (ANL), E Ben-Naim (LANL), G Grest (SNL)

D Hoffman (ex-officio, Ames)

- ◆ **Oversees center operation**
- ◆ **Apportions common resources**
 - Travel
 - Workshop
 - Evaluates outreach research proposals
 - Personnel (students, postdocs, visitors)



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Goals & Methods

Goals

- Close the gap between physics and engineering approaches to granular matter
- Develop integrated long-term experimental and computational capabilities at DOE labs

Methods

- Collaborations: Lab-Lab and Lab-partner via personnel exchange, visits
- Outreach: Workshops, visits





Second Granular Flow and Kinetics Workshop

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- ◆ Jan 18-21, 2003 at Argonne National Lab, Chicago
 - 51 participants, 30 from universities, 19 from national labs, 2 from industry
- ◆ Sessions:
 - Segregation & multiphase flows, Dense granular flows, Granular gases, Properties of static and quasi-static granular matter, Clustering and effects of fluid
- ◆ Cemented collaborative network between research groups; basis for skeletal roadmap for future research on granular flows



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Focus Areas

- ◆ **Granular gases:** dilute, collision dominated
 - Velocity statistics, correlations, kinetic theory
 - Flow equations, equation of state
- ◆ **Granular fluids:** dense, contact dominated
 - Constitutive relations, force propagation
 - Flow equations: shear, avalanches
- ◆ **Granular mixtures:** dilute and dense
 - Multiphase flow, fluid-particle coupling
 - Chains, rods

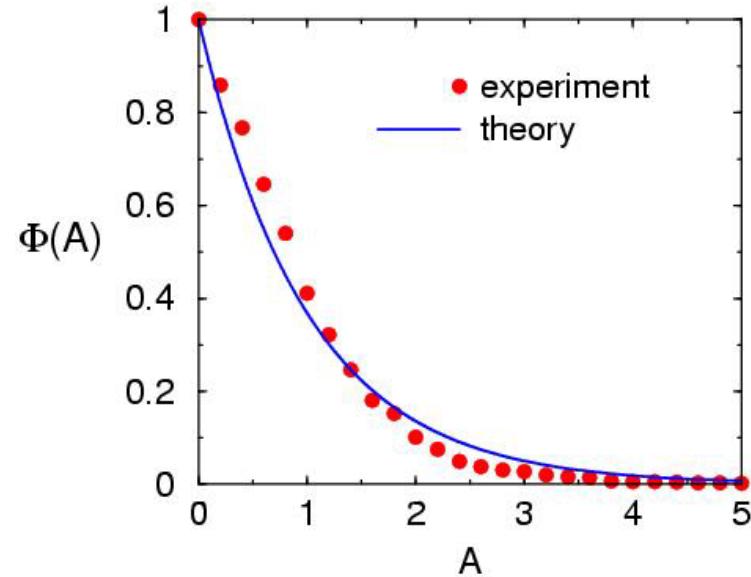




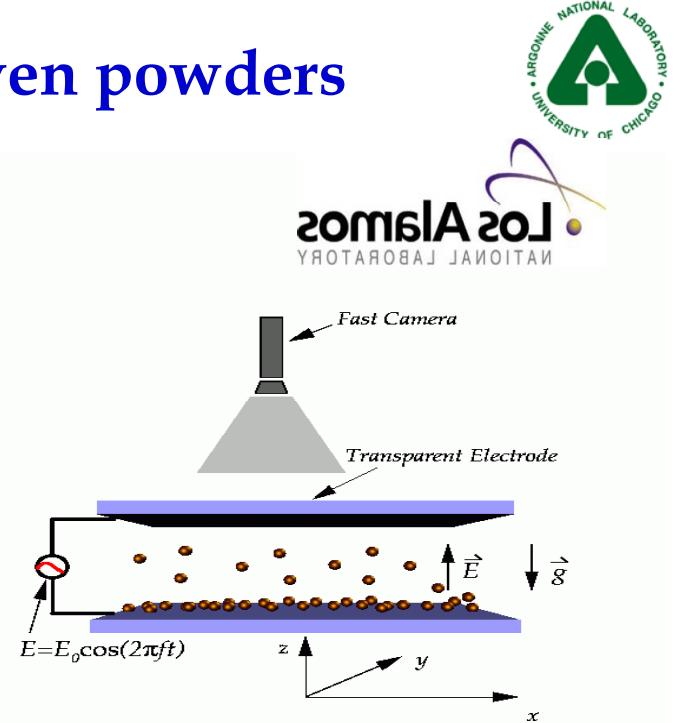
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Granular Gases: Coarsening

Experiment: electrostatically-driven powders
Theory: Exchange driven growth



$$P(A) \propto \exp(-\text{const} \times A)$$



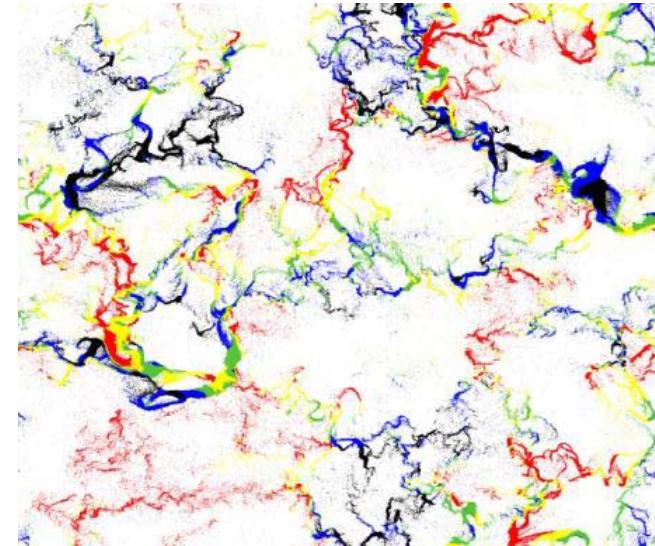
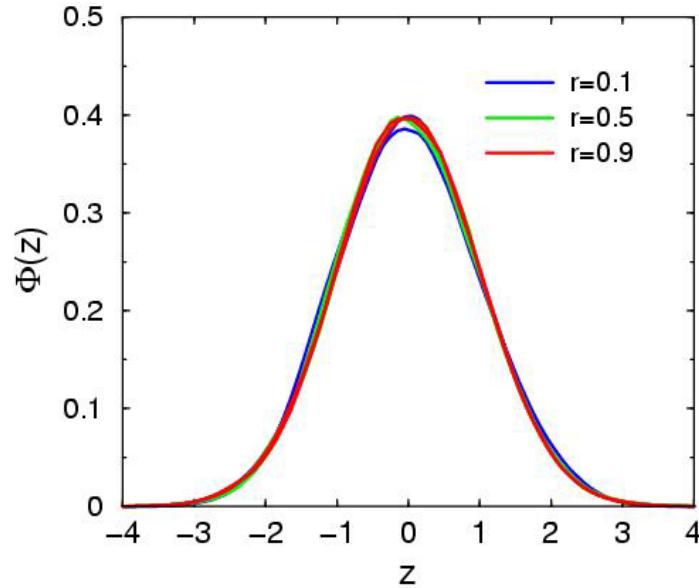


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Granular Gases: velocity statistics



- Large-scale molecular dynamics: 10^6 particles
- Uniform system develops clusters, coherent motion
- Universal velocity distribution & scale



PRL 2002

Meeting: BES 6/12/03



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Granular Flows: Hopper Simulation(MD)

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Force distribution in a flowing medium

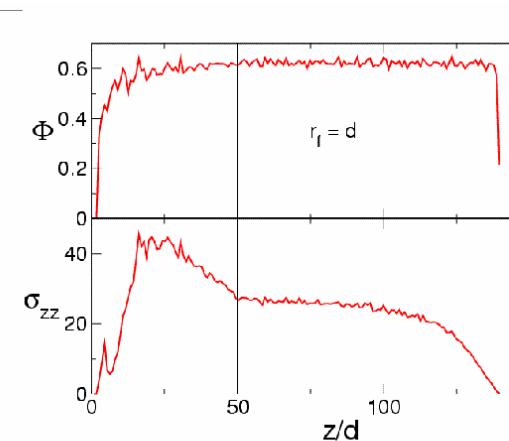
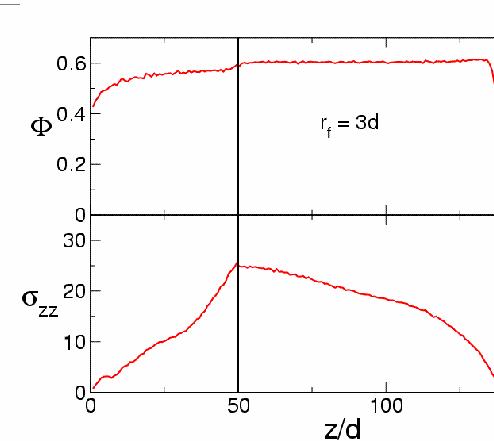
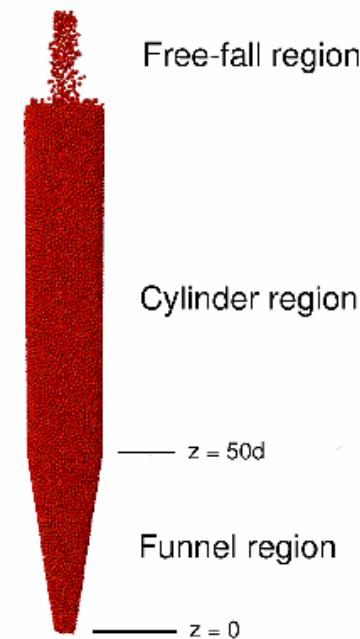


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- System changes: jamming
- Role of clustering ?

Flowing State

Jammed State



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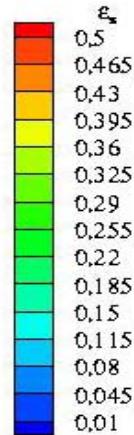
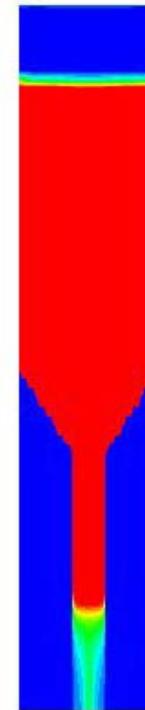
Granular Flows: Hopper Simulation(2)

Engineering devices: MFIX (NETL)
Model: Aronson & Tsimring

- Order parameter ρ
- Bridges rapid dilute flow (kinetic theory) and slow dense flow (plastic regime)
- Obeys a modeled transport eqn
- Solid stress tensor is a function of local order parameter value



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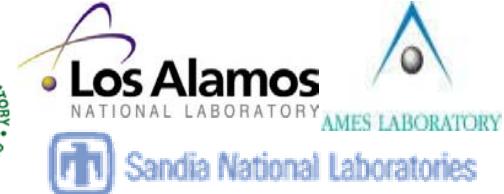
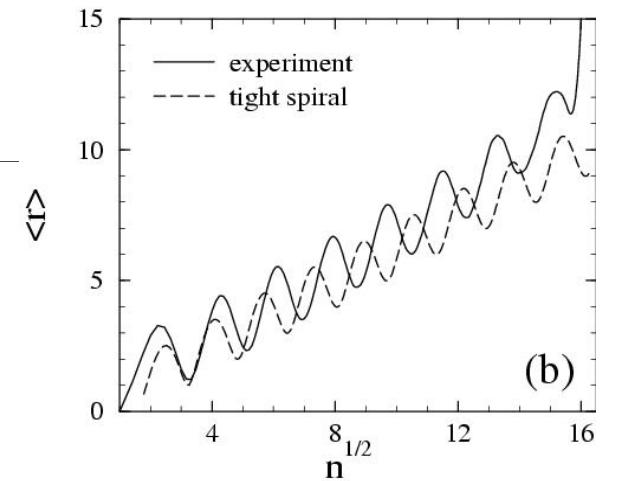
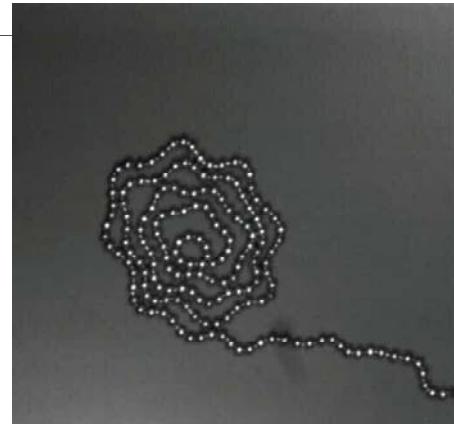
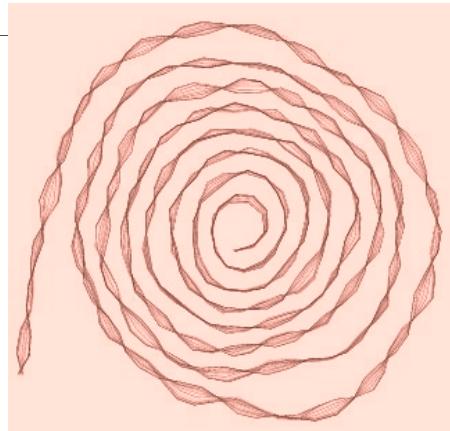




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Granular Chains: Spiral Formation

- Spirals form spontaneously
- Spiral rotates steadily, is tight
- Ratchet effect: anisotropy in chain causes rotation
- Waves: transverse dominates over lateral motion





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Center funded research projects

◆ Granular gases

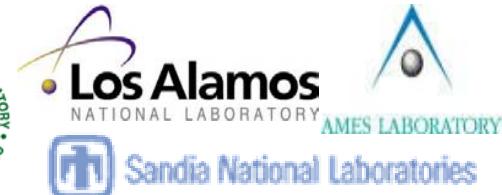
- Kinetic theory vs. MD simulations (Ames, Colorado)
- Clustering in monolayers (ANL, LANL, Kansas, Hopkins)
- Shocks & continuum theory (LANL, Hopkins)

◆ Granular fluids

- Couette shear flows: experiment, MD (SNL, Chicago)
- Linear shear flows: MC simulation (LANL, ANL)
- Step avalanches experiments (ANL, Clark U)

◆ Granular mixtures

- Air-particle interactions simulations (Ames, SNL)
- Impurities (LANL, Boston U)



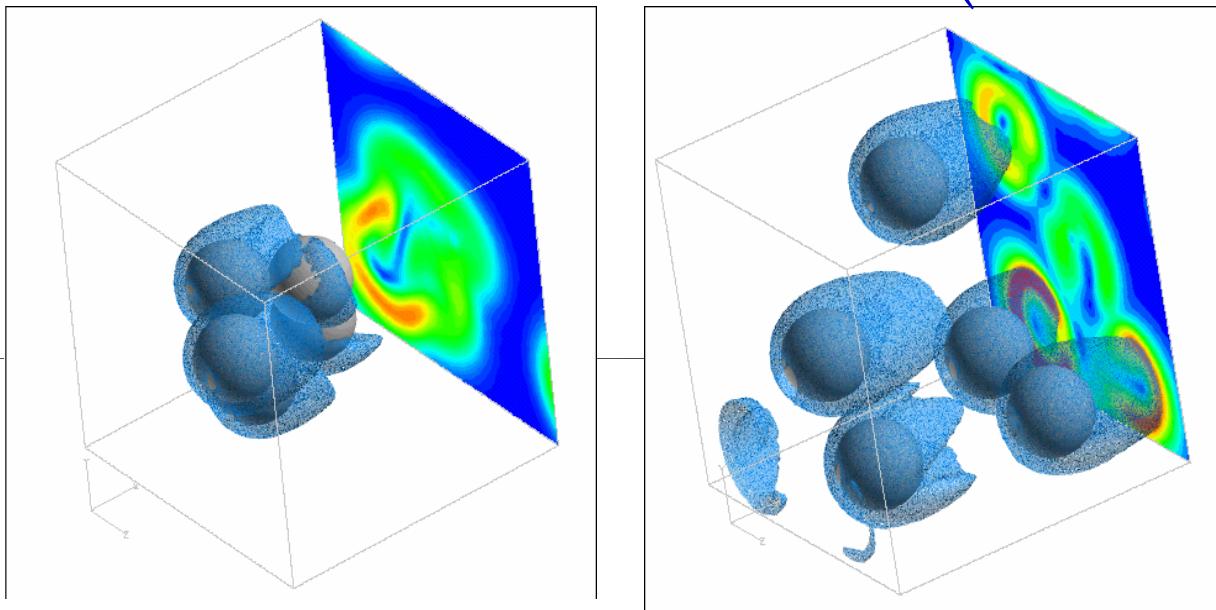
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Granular Mixtures: Multiphase flow

- Presence of fluid is important
- Direct Numerical Simulation (Mohd-Yusof)



- Steady non-turbulent flow
 $Re=100$
- Isosurfaces of vorticity
 $0.2U/D$

- Couple particles with background fluid
- Collisions: MD



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Granular Mixtures: Multiphase flow

- Sandia visit (Nov, 2002)
- Post-doc to join Ames Lab in July, 2003
- Develop hierarchy of fluid-particle simulation approaches for dense granular flows



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- LES-like spatial filtering approaches
- CFDLIB (Kashiwa, LANL) is a candidate flow solver
- Develop consistent probabilistic approach (point-process and random-field using volume-surface product measure)
- Directly extract data pertaining to unclosed terms in statistical models



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ARGONNE NATIONAL LABORATORY
UNIVERSITY OF CHICAGO



Los Alamos
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Summary

- ◆ **Goal:** Improve constitutive relations for granular materials
 - Obj 1: Close the gap between continuum & discrete descriptions
 - Obj 2: Roadmapping and outreach
- ◆ **Strategy:** Multidisciplinary approach to flow and kinetics of granular materials, theory, high-performance computing, and experiment.
- ◆ **Technical tasks:**
 - Granular Gases: velocity statistics & kinetic theory
 - Granular Fluids: constitutive relations & continuum theory
 - Granular Mixtures: multiphase flows
- ◆ **Method:** collaborations via personnel exchange & yearly workshops
- ◆ **Term:** 5 years
- ◆ **Budget:** \$300k/year



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Publications (2003)

1. **Confined granular packings: Structure, stress, and forces**, J. W. Landry, G. S. Grest, L. E. Silbert, and S. J. Plimpton, *Phys. Rev. E* **67**, 041303 (2003)
2. **Exchange Driven Growth**, E. Ben-Naim and P.L. Krapivsky. *Phys. Rev. E*, submitted (2003)
3. **Spontaneous spirals in vibrated granular chains**, R. Ecke, Z. A. Daya, M. K. Rivera, and E. Ben-Naim. *Proc. Of MRS 02 Fall Meeting*, accepted (2002).
4. **The Inelastic Maxwell Model**, E. Ben-Naim and P.L. Krapivsky. *Lecture Notes in Physics*, accepted (2003)
5. **Dynamics of Freely Cooling Granular Gases**, X. Nie, E. Ben-Naim and S.Y. Chen. *Phys. Rev. Lett.*, **89**, 204301, (2002)
6. **Impurity in a Maxwellian Unforced Granular Fluid**, E. Ben-Naim and P.L. Krapivsky. *Eur. Phys. Jour. E* **8**, **507** (2002)
7. **Inontrivial velocity distributions in Inelastic Gases**, E. Ben-Naim and P.L. Krapivsky. *Phys. Rev. E*, **66**, 025102 (2002)



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Publications (2003)

8. **Molecular dynamics simulations and continuum theory of partially fluidized shear granular flows**, Dmitri Wolfson, Lev S. Tsimring, and Igor S. Aranson, *Phys. Rev. Lett.*, to appear (2003)
9. **Model of coarsening and vortex formation in vibrated granular rods**, Igor S. Aranson and Lev S. Tsimring, *Phys. Rev. E* (Statistical, Nonlinear, and Soft Matter Physics), Volume 67, Issue 2, Article 021305
10. **Velocity fluctuations in electrostatically driven granular media**, I. S. Aranson and J. S. Olafsen Physical Review E (Statistical, Nonlinear, and Soft Matter Physics), Volume 66, Issue 6, Article 061302
11. **Coarsening of granular clusters: Two types of scaling behaviors**, M. V. Sapozhnikov, I. S. Aranson, and J. S. Olafsen, *Phys. Rev. E* (Statistical, Nonlinear, and Soft Matter Physics), Volume 67, Issue 1, Article 010302
12. **Vortices in vibrated granular rods**, Daniel L. Blair, T. Neicu, and A. Kudrolli Physical Review E (Statistical, Nonlinear, and Soft Matter Physics) *Phys. Rev. E*, **67**, 031303 (2003)



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University and industrial partners

- ❖ S Nagel, H Jaeger, L Kadanoff (U Chicago)
- ❖ L Tsimring (UCSD)
- ❖ J Olafsen (U Kansas)
- ❖ B Behringer (Duke)
- ❖ A Kudrolli (Clark U)
- ❖ S Chen (Johns Hopkins)
- ❖ P Krapivsky (Boston U)
- ❖ J Stringer (EPRI)
- ❖ T Halsey, T Mason, D Ertas (ExxonMobil)
- ❖ E Fukushima (New Mexico Resonance)





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DOE Lab programs

LAB	CORE PROGRAM		GLUE PROGRAM			
	program/people	k\$	area	k\$	people	partners
Ames	multiphase flow 2 staff, 2 students	250 BES	fluids mixtures	110*	2 students	colorado iowa st.
ANL	granular physics 3 staff, 2 postdocs	750 BES	gases fluids	75	½ postdoc student	ucsd kansas
LANL	granular media 4 staff, 4 postdocs	400 BES+	gases mixtures	70	½ postdoc student	boston hopkins
SNL	ceramics 2 staff, 2 postdocs	200 BES	fluids mixtures	45	½ postdoc student	exxon chicago
total	11 senior/10 junior	1600		300	7 junior	



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FY02 Budget: 300K

Lab	PI	Gases	Fluids	Mixtures	Outreach	Total
Ames	Hoffman		20	25	65	110
ANL	Aronson	45	40			75
LANL	Hurd	35		35		70
SNL	Grest		45			45
Total		80	105	60	65	300

Outreach	Annual workshop	Travel	University collaborations	Total
Funding	15	10	40	65